# Ouercetin

Quercetin is a plant flavonol from the flavonoid group of polyphenols. It is found in many fruits, vegetables, leaves, seeds, and grains; red onions and kale are common foods containing appreciable content of quercetin. [2] Quercetin has a bitter flavor and is used as an ingredient in dietary supplements, beverages, and foods.

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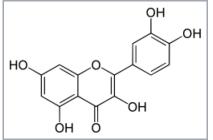
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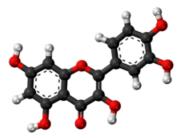
### Occurrence

Quercetin is a flavonoid widely distributed in nature. [2] The name has been used since 1857, and is derived from *quercetum* (oak forest), after *Quercus*.<sup>[3][4]</sup> It is a naturally occurring polar auxin transport inhibitor.<sup>[5]</sup>

Quercetin is one of the most abundant dietary flavonoids, [2][6] with an average daily consumption of 25–50 milligrams.<sup>[7]</sup>

### Quercetin





#### **Names**

Pronunciation /'kwa:rsitin/

**IUPAC** name

2-(3,4-dihydroxyphenyl)-3,5,7trihydroxy-4H-chromen-4-one

#### Other names

5,7,3',4'-flavon-3-ol, Sophoretin, Meletin, Quercetine, Xanthaurine, Quercetol, Quercitin, Quertine, Flavin meletin

### **Identifiers**

**CAS Number** 117-39-5 (http://w ww.commonchemi stry.org/ChemicalD etail.aspx?ref=117 -39-5) 🗸 6151-25-3 (http:// www.commonche mistry.org/Chemic alDetail.aspx?ref= 6151-25-3) (Quercetin dihydrate)[1] x 3D model Interactive image

# (JSmol)

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Foods	Quercetin (mg/100g)
capers, raw	234 <sup>[6]</sup>
capers, canned	173 <sup>[6]</sup>
dock like sorrel	86 <sup>[6]</sup>
radish leaves	70 <sup>[6]</sup>
carob fiber	58 <sup>[6]</sup>
dill	55 <sup>[8]</sup>
cilantro	53 <sup>[6]</sup>
Hungarian wax pepper	51 <sup>[6]</sup>
fennel leaves	49 <sup>[6]</sup>
onion, red	32 <sup>[6]</sup>
radicchio	32 <sup>[6]</sup>
watercress	30[6]
kale	23 <sup>[6]</sup>
chokeberry	19 <sup>[6]</sup>
bog blueberry	18 <sup>[6]</sup>
cranberry	15 <sup>[6]</sup>
lingonberry	13 <sup>[6]</sup>
plums, black	12 <sup>[6]</sup>

In red onions, higher concentrations of quercetin occur in the outermost rings and in the part closest to the root, the latter being the part of the plant with the highest concentration.<sup>[9]</sup> One study found that <u>organically grown</u> tomatoes had 79% more quercetin than non-organically grown fruit.<sup>[10]</sup> Quercetin is present in various kinds of honey from different plant sources.<sup>[11]</sup>

## **Biosynthesis**

In plants, phenylalanine is converted to  $\underline{4}$ -coumaroyl-CoA in a series of steps known as the general phenylpropanoid pathway using phenylalanine ammonia-lyase, cinnamate- $\underline{4}$ -hydroxylase, and  $\underline{4}$ -coumaroyl-CoA-ligase. One molecule of  $\underline{4}$ -coumaroyl-CoA is added to three molecules of  $\underline{malonyl-CoA}$  to form tetrahydroxychalcone using 7,2'-dihydroxy- $\underline{4}$ '-methoxyisoflavanol synthase. Tetrahydroxychalcone is then converted into  $\underline{naringenin}$  using chalcone isomerase.

Naringenin is converted into <u>eriodictyol</u> using flavanoid 3'-hydroxylase. Eriodictyol is then converted into <u>dihydroquercetin</u> with flavanone 3-hydroxylase, which is then converted into quercetin using flavonol synthase.<sup>[12]</sup>

## **Glycosides**

Quercetin is the aglycone form of a number of other flavonoid glycosides, such as <u>rutin</u> and quercitrin, found in <u>citrus</u> fruit, <u>buckwheat</u> and onions. Quercetin forms the glycosides quercitrin and <u>rutin</u> together with <u>rhamnose</u> and <u>rutinose</u>, respectively. Likewise guaijaverin is the 3-O-arabinoside, <u>hyperoside</u> is the 3-O-galactoside, <u>isoquercitin</u> is the 3-O-glucoside and <u>spiraeoside</u> is the 4'-O-glucoside. <u>CTN-986</u> is a quercetin derivative found in cottonseeds and cottonseed oil. Miquelianin is the quercetin 3-O-B-D-glucuronopyranoside.

### **Rutin degradation pathway**

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ChEBI	CHEBI:16243 (http s://www.ebi.ac.uk/c hebi/searchId.do?c hebiId=16243) *
ChEMBL	ChEMBL50 (https:// www.ebi.ac.uk/che mbldb/index.php/c ompound/inspect/ ChEMBL50) <
ChemSpider	4444051 (http://w ww.chemspider.co m/Chemical-Struct ure.4444051.html)
DrugBank	DB04216 (https://www.drugbank.ca/drugs/DB04216)
ECHA InfoCard	100.003.807 (http s://echa.europa.eu/ substance-informa tion/-/substanceinf o/100.003.807)
IUPHAR/BPS	5346 (http://www.g uidetopharmacolo gy.org/GRAC/Ligan dDisplayForward?t ab=summary&liga ndId=5346)
KEGG	C00389 (https://w ww.kegg.jp/entry/C 00389) ✓
PubChem <u>CID</u>	5280343 (https://p ubchem.ncbi.nlm.n ih.gov/compound/5 280343)
UNII	9IKM0I5T1E (http s://fdasis.nlm.nih.g ov/srs/srsdirect.js p?regno=9IKM0I5T 1E) *
CompTox Dashboard (EPA)	DTXSID4021218 (h ttps://comptox.ep a.gov/dashboard/D TXSID4021218)
InChl	

9(18)3-6/h1-5,16-19,21H ✓ Key: REFJWTPEDVJJIY-UHFFFAOYSA-N ✓ The enzyme quercitrinase can be found in Aspergillus flavus. [14] This enzyme hydrolyzes the glycoside quercitrin to release quercetin and L-rhamnose. It is an enzyme in the rutin catabolic pathway.[15]

## **Pharmacology**

### **Pharmacokinetics**

The bioavailability of quercetin in humans is low and highly variable (0-50%), and it is rapidly cleared with an elimination half-life of 1-2 hours after ingesting quercetin foods or supplements. [16] Following dietary ingestion, quercetin undergoes rapid and extensive metabolism that makes the biological effects presumed from *in vitro* studies unlikely to apply *in* vivo.[17][18]

#### Metabolism

In rats, quercetin did not undergo any significant phase I metabolism.<sup>[19]</sup> In contrast, quercetin did undergo extensive phase II (conjugation) to produce metabolites that are more polar than the parent substance and hence are more rapidly excreted from the body. The meta-hydroxyl group of catechol is methylated by catechol-O-methyltransferase. Four of the five hydroxyl groups of quercetin are glucuronidated by UDP-glucuronosyltransferase. The exception is the 5-hydroxyl group of the flavonoid ring which generally does not undergo glucuronidation. The major metabolites of orally absorbed quercetin are quercetin-3-glucuronide, 3'-methylquercetin-3-glucuronide, and quercetin-3'-sulfate. [19][20]

### In vitro pharmacology

Quercetin has been reported to inhibit the oxidation of other molecules and hence is classified as an antioxidant. [17][20] It contains a polyphenolic chemical substructure that stops oxidation by acting as a scavenger of free radicals that are responsible for oxidative chain reactions. [21]

Ouercetin also activates or inhibits the activities of a number of proteins. [22] For example, quercetin is a non-specific protein kinase enzyme inhibitor. [17][20] Ouercetin has also been reported to have estrogenic (female sex hormone-like) activities by activating estrogen receptors. Quercetin activates both estrogen receptor alpha (ERα) and beta (ERβ)<sup>[23]</sup> with binding IC<sub>50</sub> values of 1015 nM and 113 nM, respectively. Hence quercetin is somewhat ERβ selective (9 fold) and is roughly two to three orders of magnitude less potent than the endogenous estrogenic hormone 17β-estradiol.<sup>[24][25]</sup> In human breast cancer cell lines, quercetin has also been found to act as an agonist of the G protein-coupled estrogen receptor (GPER).<sup>[26]</sup>

### Health claims

Quercetin has been studied in basic research and small clinical trials. [28][2][29][30] While quercetin supplements have been promoted for the treatment of cancer and various other diseases, [31] there is no evidence that quercetin (via supplements or in food) is useful to treat cancer<sup>[32]</sup> or any disease.[2][33]

The US Food and Drug Administration has issued warning letters to several manufacturers advertising on their product labels and websites that quercetin product(s) can be used to treat diseases. [34][35] The FDA regards such quercetin advertising and products as unapproved – with unauthorized health claims concerning the anti-disease products - as defined by "sections 201(g) (1)(B) and/or  $\overline{201}$  (g)(1)(C) of the Act [21 U.S.C. § 321(g)(1)(B) and/or 21 U.S.C. § 321(g)(1)(C)] because they are intended for use in the diagnosis, cure, mitigation, treatment, or prevention of disease", [34][35] conditions which were not met by the manufacturers.

InChI=1/C15H10O7/c16-7-4-10(19)12-11(5 -7)22-15(14(21)13(12)20)6-1-2-8(17)9(1 8)3-6/h1-5,16-19,21H Key: REFIWTPEDVIJIY-UHFFFAOYAW

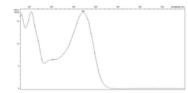
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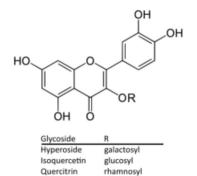
Properties	
Chemical formula	C <sub>15</sub> H <sub>10</sub> O <sub>7</sub>
Molar mass	302.236 g/mol
Appearance	yellow crystalline powder <sup>[1]</sup>
Density	1.799 g/cm <sup>3</sup>
Melting point	316 °C (601 °F; 589 K)
Solubility in water	Practically insoluble in water; soluble in aqueous alkaline solutions <sup>[1]</sup>

Except where otherwise noted, data are given for materials in their standard state (at 25 °C [77 °F], 100 kPa).

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UV visible spectrum of quercetin, with lambda max at 369 nm.



3-O-Glycosides of guercetin

### Safety

In preliminary human studies, oral intake of quercetin in doses up to one gram per day over three months did not cause <u>adverse</u> effects.<sup>[2]</sup> The safety of using quercetin in dietary supplements during pregnancy and lactation has not been established.<sup>[2]</sup>

### See also

- List of ineffective cancer treatments
- Flavonol 3-sulfotransferase
- Phenolic compounds in wine
- Phytochemical
- Quercetin 2,3-dioxygenase
- Quercetin 3-O-methyltransferase
- Quercetin-3-sulfate 3'sulfotransferase
- Quercetin-3-sulfate 4'sulfotransferase
- Quercetin-3,3'-bissulfate7-sulfotransferase

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